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THEORETICAL TRANSPORT STUDIES OF NON-EQUILIBRIUM CARRIERS DRIVEN BY HIGH ELECTRIC FIELDS

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Final Report

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14. ABSTRACT:
This work examines quantum transport in nanowires with several different formalisms. The Boltzmann equation based theory of Lyo and Huang is able to incorporate many different kinds of scattering and make interesting predictions but found absent in it a simple way of providing physical understanding of its effects. The STM theory of Kenkre, Biscarini, and Bustamante incorporates incoherent scattering in a much simpler way, but difficulties arise when the motion is fully coherent. Wigner functions, which are quasi-probability distributions defined on phase space, are appealing because of the conceptual similarity to classical transport theory. Calculated the Wigner function for ballistic 1D conductors and show that the current reduces to the Landauer result, but incorporating boundary conditions correctly in more complicated cases remains a problem to complete. Found the transmission formalism to be quite useful for simpler systems with elastic scattering when the motion is fully coherent and have provided analysis of interactions of the conductor with a bath represented in a simple manner by harmonic vibrations.

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1 Introduction

The work on this project was performed by the graduate research assistant Alden Astwood in collaboration with the P.I. V. M. Kenkre. Our study was motivated by the work of Lyo and Huang in which they analyzed the effects of various types of scattering in single and double quantum wires using a Boltzmann equation formalism [1, 2, 3, 4]. In particular, one of Lyo and Huang's interesting predictions is that the conductance as a function of a magnetic field is quite different when there is scattering as opposed to when the motion is ballistic.

In the past few decades it has become possible to fabricate high mobility transistors which are small enough that electrons are able to maintain a definite phase as they move through the junction. Non-traditional analysis becomes therefore important to describe quantum effects adequately. Commonly studied systems are GaAs-AlGaAs heterostructures, in which the difference in bandgap of the two materials causes a high mobility two-dimensional electron gas (2DEG) to form at the interface. This effect is described in many solid state textbooks, e.g. see [5]. Lithography techniques can be used to etch a gate onto the structure. This allows the effective width of the junction to be controlled. Devices thus constructed are known as nanowires, quantum wires, or quantum point contacts. Because of the low amount of scattering in these structures, the conductance as a function of gate voltage or transverse magnetic field can be quite different than what is predicted by Ohm's law. Many formalisms have been developed to analyze transport in quantum wires, most prominently the transmission formalism developed by Landauer and others [6, 7, 8, 9, 10, 11].

We pursued in this project a variety of theoretical approaches to the description of quantum transport in nanowires. In previous reporting periods we considered the application of a transport theory developed by Kenkre, Biscarini, and Bustamante for analyzing scanning tunneling microscopy (STM) images to transport in quantum wires [12, 13, 14, 15, 16, 17]. Incoherent scattering effects are incorporated in the theory in a particularly simple way through the stochastic Liouville equation (SLE). In the simplest form of that theory, a single parameter α controls the strength of incoherent scattering effects, and adjusting this parameter is a quick usable way to analyze the transport behavior for different amounts of scattering in the conductor. Within the time period we devoted to the STM theory in this project we could not construct a complete theoretical tool based on that formalism because of level broadening issues. These issues arise because of the coupling to the contacts. We have discussed these issues in a previous report as this broadening limits the amount of current that can be forced through the conductor. It still remains unclear to us how to incorporate these broadening effects into the STM theory.

Modeling the transport using Wigner functions is another avenue we have pursued in this work. Analogous to the classical distribution function, a Wigner function is a quantity defined on phase space, but unlike the classical distribution function, the Wigner function still contains complete information about the quantum state of the system [18, 19]. The Wigner function obeys an equation of motion which is conceptually similar to the classical Boltzmann equation. In an earlier report we calculated the Wigner functions in the steady state in a quasi-1D quantum wire for two different types of confinement. Motivated by our desire to understand scattering processes in quantum wires in a simple way, in the final reporting period we focussed on applying the existing transmission formalism to successively more complicated systems as shown below. We hope that our results will be useful to further investigations on this problem.

2 Lyo and Huang Boltzmann Equation Solution

As a starting point, Lyo and Huang take a Boltzmann equation [1, 2, 3, 4],

$$v_j + \frac{2\pi}{\hbar}\sum_j |V_{j',j}|^2 (g_{j'} - g_j)\delta(\mathcal{E}_j - \mathcal{E}_{j'}) = 0. \tag{1}$$

Here the v_j's and $\mathcal{E}_j$'s are respectively group velocities and energies of electrons in the jth subband, g_j is the nonequilibrium part of the distribution function, and the $|V_{j',j}|$'s represent scattering matrix elements. This Boltzmann equation is then formally solved, and their expression for the conductance is

$$G = -\frac{2q^2}{hL_y}\int_0^\infty d\mathcal{E}[-f_0'(\mathcal{E})]\mathbf{S}^\dagger \mathbf{U}^{-1}\mathbf{S} \tag{2}$$

where $\mathbf{S}$ is a vector which contains the signs of the velocities v_j, and $\mathbf{U}$ is a matrix with elements related to the scattering matrix elements $|V_{j',j}|^2$. Lyo and Huang have shown that indeed this reduces to the well known Landauer result if the motion is ballistic, and they have used this approach to analyze the effects of different kinds of scattering.

One result of theirs which we have found particularly interesting is that the behavior of the conductance as a function of magnetic field is quite different from the ballistic result when the wires are rough or dirty. From the published work of Lyo and Huang we have not been able to understand *physically* how the conductance behaves if the amount of scattering is increased or decreased by given amounts although they certainly have provided a detailed formalism for calculation.

3 Kenkre et al. STM Theory

The transport theory by Kenkre, Biscarini, and Bustamante [12, 13, 14, 15, 16, 17] implements incoherent scattering in a particularly simple way. We pursued this approach because of the appealing possibility of understanding how different amounts of incoherent scattering affect the conductance. Their expression for the resistance is

$$R = \frac{1}{q^2 n_e}\left\{\frac{\int_0^\infty dt[\Pi_{SS}(t) - \Pi_{ST}(t)]}{\left(\frac{\Delta\eta_S^{\mathrm{th}}}{\mu-\mu_S}\right)} + \frac{\int_0^\infty dt[\Pi_{TT}(t) - \Pi_{TS}(t)]}{\left(\frac{\Delta\eta_T^{\mathrm{th}}}{\mu-\mu_T}\right)}\right\} \tag{3}$$

where n_e is the number of electrons in the junction, $\Delta\eta$'s are differences from equilibrium populations, the μ's are chemical potentials, and the Π's are probability propagators. The probability propagators can be found, for example, by solving a Master equation if the motion is fully incoherent, or a stochastic Liouville equation (SLE), equivalent to a generalized Master equation, if the motion is partially coherent. One form of the SLE adds a term to the Liouville-von Neumann equation which causes off-diagonal elements of the density matrix to decay to their thermal values [20],

$$\frac{\partial\rho_{mn}}{\partial t} = \frac{1}{i\hbar}[H,\rho]_{mn} - \alpha(1-\delta_{mn})(\rho_{mn} - \rho_{mn}^{\mathrm{th}}) \tag{4}$$

where α is a parameter which controls the amount of coherence. Exact propagators for some systems are known and may be found in the literature (see for example [21] and [22]).

One issue that arises with this approach is that when the transport is fully coherent, the propagators are periodic for a finite system, and certain integrals, like those in equation (3), are divergent. However, when the transport is fully coherent, level broadening effects due to coupling to infinite sized contacts limit the maximum amount of current that can be forced through the junction, and the resistance is finite [23]. Discussion of broadening effects in a one-level system has been included in previous reports. While it is still not clear to us how to incorporate broadening while maintaining this formulation in terms of the probability propagators for multi-level systems, one of the avenues we would pursue if we had more time would be to consider the idealization of infinite systems to avoid the technical problems we encountered.

4 Wigner Function Approach

Using Wigner functions to model transport is desirable because of the conceptual similarity to classical transport theory. Unlike the classical distribution function, it makes sense to talk about the density matrix as a function of two position variables (i.e. $\rho(\mathbf{x}, \mathbf{x}', t) \equiv \langle \mathbf{x}|\rho(t)|\mathbf{x}'\rangle$) or two momentum variables, (i.e. $\rho(\mathbf{x}, \mathbf{x}', t) \equiv \langle \mathbf{x}|\rho(t)|\mathbf{x}'\rangle$), but it does not make sense to talk about the density matrix as a function on phase space. However, it is possible to transform $\rho(\mathbf{x}, \mathbf{x}', t)$ to center of mass and relative coordinates, then perform a Fourier transform on the relative coordinate. The resulting quantity, the Wigner function, is now a function defined on phase space, and since the transformation is invertible, the Wigner function still contains all the information about the quantum state of the system that the density matrix does.

The Wigner W function can be defined (in d dimensions) as [18, 19, 24, 25]

$$W(\mathbf{x}, \mathbf{p}, t) = \frac{1}{h^d} \int d\mathbf{s} e^{-i\mathbf{p}\cdot\mathbf{s}/\hbar} \langle \mathbf{x} + \mathbf{s}/2|\rho(t)|\mathbf{x} - \mathbf{s}/2\rangle. \tag{5}$$

Transforming the von Neumann equation for the evolution of the density, the time evolution of the Wigner function can be shown to obey

$$\frac{\partial W}{\partial t} = -\frac{\mathbf{p}}{m} \cdot \frac{\partial W}{\partial \mathbf{x}} + \int d\mathbf{p}' \chi(\mathbf{x}, \mathbf{p}') W(\mathbf{x}, \mathbf{p} + \mathbf{p}', t) \tag{6}$$

where χ is

$$\chi(\mathbf{x}, \mathbf{p}') \equiv \frac{1}{h^d} \int d\mathbf{s} \sin(\mathbf{p}' \cdot \mathbf{s}/\hbar)[U(\mathbf{x} + \mathbf{s}/2) - U(\mathbf{x} - \mathbf{s}/2)]. \tag{7}$$

This is similar to the classical Boltzmann equation, but because of interference effects the second term is nonlocal.

In the previous reporting period, we showed that the Wigner function for a quasi-1D ballistic conductor in the steady state is

$$W(\mathbf{x}, \mathbf{p}) = \frac{1}{h} \sum_n [\Theta(p_y) f(\mathcal{E}_{n,p_y/\hbar} - \mu_L) + \Theta(-p_y) f(\mathcal{E}_{n,p_y/\hbar} - \mu_R)] W_n(x, p_x) \tag{8}$$

where Θ is the step function, $\mathcal{E}_{n,p_y/\hbar}$ is the energy of a state which is in the nth excited state of the confinement potential and has momentum p_y in the y direction, μ_L and μ_R are the electrochemical potentials of the left and right contacts, and $W_n(x, p_x)$ is the Wigner function corresponding to the nth excited state of the confinement potential. Using the expression

$$\langle O \rangle = \int\int d\mathbf{x}d\mathbf{p}O(\mathbf{x}, \mathbf{p})W(\mathbf{x}, \mathbf{p}), \tag{9}$$

where $O(\mathbf{x}, \mathbf{p})$ is the Wigner-Weyl transform of an observable O, to calculate the current, and taking the low bias, low temperature limit, we were able to recover the Landauer result for the quantized conductance.

Some authors have already done some work using Wigner functions to study quantum transport in resonant tunneling diodes; e.g. see [26, 27]; however, as discussed in [25], one difficulty with applying the Wigner function representation for more complicated systems is correctly incorporating open boundary conditions into the problem.

5 Transmission Formalism

The transmission formalism developed by Landauer and others [6, 7, 8, 9, 10, 11] has been a popular tool for calculating current in quantum wires and other mesoscale devices.

In order for current to flow through a conductor, it must be connected to at least two contacts. One contact is assumed to be interacting with a reservoir at electrochemical potential μ_1, and the other is interacting with a reservoir at electrochemical potential μ_2. This difference in electrochemical potentials causes electrons to flow from one contact to the other through the conductor. Landauer and others have shown that when the transport is coherent (i.e. there are no phase-breaking scattering processes), the current in the conductor is related to the transmission function $T(E)$. At finite temperature, the current is [28, 23]

$$I = \frac{2q}{h}\int_{-\infty}^{\infty} M(E)T(E)[f_1(E) - f_2(E)]dE \tag{10}$$

where $f_1(E)$ and $f_2(E)$ are the Fermi functions of the two contacts and $M(E)$ is the number of modes with energy less than E. The transmission function (per mode) $T(E)$ is defined to be the probability that an electron injected into one contact with energy E will reach the other contact.

At low bias and low temperature, this reduces to

$$I \approx \frac{2q^2}{h}VMT \tag{11}$$

so the conductance is

$$G = \frac{I}{V} = \frac{2q^2}{h}MT. \tag{12}$$

This simple relationship has been used in the literature to calculate currents in mesoscale devices with high mobilities. In a quasi-1d ballistic conductor ($T = 1$), the number of modes M can be varied by adjusting the voltage of a gate or the strength of a transverse magnetic field. This leads to a kind of quantization of the conductance, which has been experimentally measured by van Wees et al. and others [29, 30, 31].

The Landauer formalism can also be expanded to include multi-terminal measurements, and phase-breaking scattering processes can be included phenomenologically by connecting a terminal

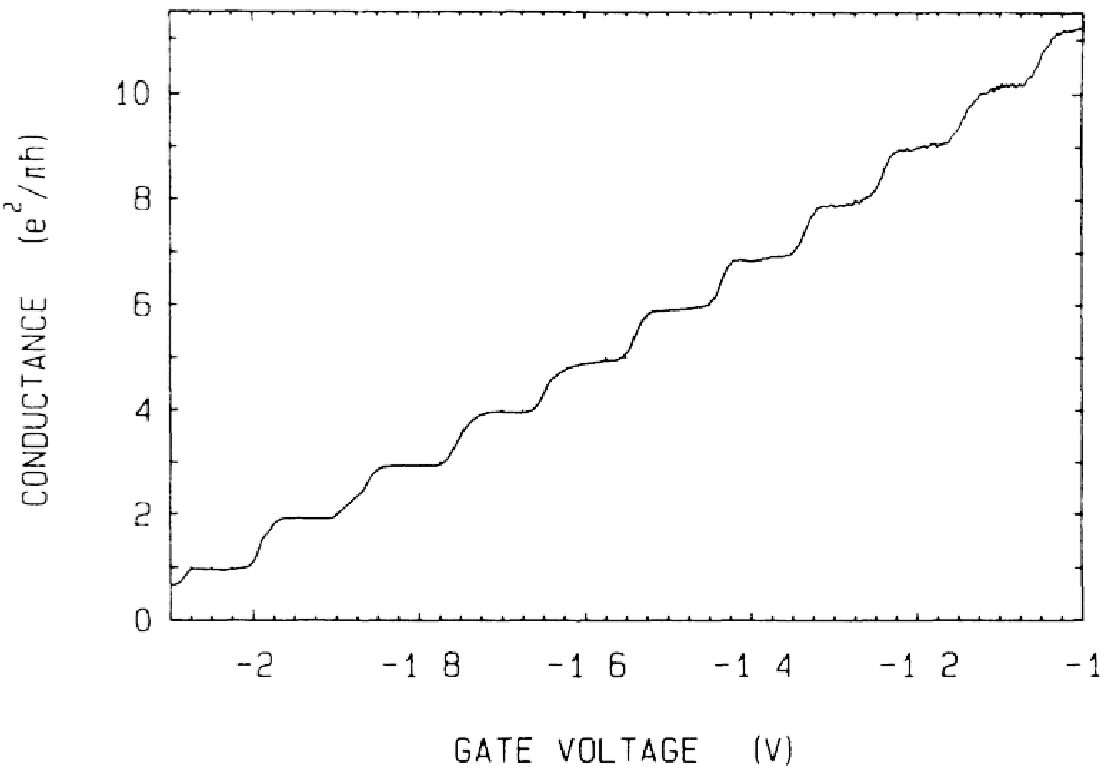

Figure 1: Experimental measurement of quantized conductance by van Wees et al. [30].

which extracts electrons from the conductor and reinjects them with a different phase (see e.g. discussions in [28]).

It is sometimes useful to express the transmission $T(E)$ in terms of the Green's function through use of the Fisher-Lee relation [32]. When the conductor is coupled to two contacts, the Green's function for the conductor subsystem becomes [28, 23]

$$G(E) = [E - H_c - \Sigma_1(E) - \Sigma_2(E)]^{-1} \tag{13}$$

where H_c is the Hamiltonian of the isolated conductor, and Σ_1 and Σ_2 are non-Hermitian and energy dependent self energies which arise from the coupling to the contacts. The self energy $\Sigma_1(E)$ is related to the (retarded) Green's function of the isolated contact, $G_1 \equiv [E - H_1]^{-1}$, and the coupling matrix τ_1 which connects the contact to the conductor:

$$\Sigma_1 \equiv \tau_1 G_1 \tau_1^\dagger. \tag{14}$$

Σ_2 is similarly defined for the second contact. Once the self energies and $G(E)$ are known, the transmission (times the number of modes) can be calculated from the relation [28, 23]

$$M(E)T(E) = \mathrm{Tr}\{\Gamma_1 G \Gamma_2 G^\dagger\} \tag{15}$$

where the trace runs over conductor states and Γ_1 and Γ_2 are related to the self energies by $\Gamma_1 \equiv i(\Sigma_1 - \Sigma_1^\dagger)$ and $\Gamma_2 \equiv i(\Sigma_2 - \Sigma_2^\dagger)$.

This relationship also connects the Landauer transmission theory to the more general non-equilibrium Green's function formalism developed by Keldysh, Kadanoff and Baym, and others [33, 34].

6 Analytic Transmission Calculations for Tight Binding Systems

We chose to examine several models within the context of the transmission theory in order to help us better understand how scattering affects the conductance. We begin below with a 1-level conductor connected to two semi-infinite contacts. Next, we consider a 2-level conductor with both energy levels connected to both contacts and compare with the one level system. The result is then generalized to N degenerate levels, each connected to both contacts. Finally, we consider a single level conductor which is interacting with a harmonic oscillator.

6.1 1-Level Conductor

The problem of single impurity scattering has already been worked out in the literature (in particular see [35] or the discussions in [28] or [23]), but we reproduce the result here for comparison.

We consider a conductor consisting of a single site with energy ϵ_0. The conductor is coupled to two semi-infinite 1D tight binding chains with nearest neighbor interaction strength V. The strength of the coupling from conductor to contacts is ηV. The total Hamiltonian is

$$H = H_L + H_R + H_c + \tau_L + \tau_L^\dagger + \tau_R + \tau_R^\dagger \tag{16}$$

where H_L and H_R are the Hamiltonians for the isolated left and right contacts, H_c is the Hamiltonian for the isolated conductor, and τ_L and τ_R represent the coupling between conductor and contacts,

$$H_L \equiv V \sum_{m<-1} \left[|m\rangle\langle m+1| + |m+1\rangle\langle m|\right], \tag{17}$$

$$H_R \equiv V \sum_{m>0} \left[|m\rangle\langle m+1| + |m+1\rangle\langle m|\right], \tag{18}$$

$$H_c \equiv \epsilon_0 |0\rangle\langle 0|, \tag{19}$$

$$\tau_L \equiv \eta V |0\rangle\langle -1|, \tag{20}$$

$$\tau_R \equiv \eta V |0\rangle\langle 1|. \tag{21}$$

To calculate the transmission $T(E)$ we consider a wavefunction consisting of an incident wave from the left, an outgoing reflected wave on the left, and a transmitted wave on the right:

$$\langle m|\psi\rangle = \begin{cases} e^{ikm} + re^{-ikm} & \text{for } m < 0 \\ \psi_0 & \text{for } m = 0 \\ te^{ikm} & \text{for } m > 0 \end{cases}. \tag{22}$$

Enforcing $H|\psi\rangle = E|\psi\rangle$, we must have

$$T(E) = |t|^2 = \frac{\hbar^2 v^2(E)}{\frac{[E(1-\eta^2)-\epsilon_0]^2}{\eta^4} + \hbar^2 v^2(E)} \tag{23}$$

where

$$\hbar^2 v^2(E) \equiv 4V^2 - E^2 = 4V^2 \sin^2 k. \tag{24}$$

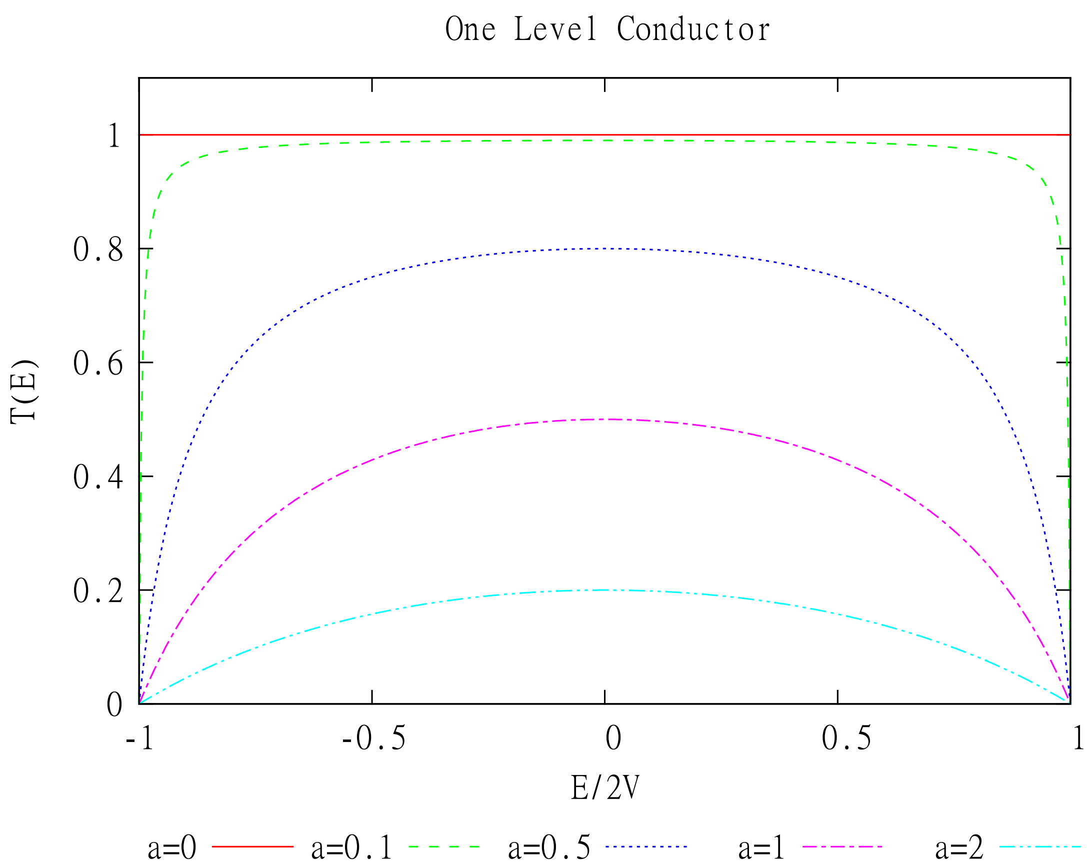

Figure 2: Transmission versus energy for the one level conductor with $\eta = 1$ for different values of $a \equiv \epsilon_0/2V$

To illustrate the equivalence of this procedure and the Green's function method, we note that the Green's function for the semi-infinite tight binding contacts can be obtained from the well known expression for the infinite chain (see [36]) using the method of images. Assuming we are within the band, $-2V < E < 2V$, the resulting self-energies are

$$\Sigma_L(E) = \Sigma_R(E) = \eta^2 V e^{-i|\theta|} |0\rangle\langle 0| \tag{25}$$

where $\cos\theta = E/2V$ and θ is chosen to be between $-\pi$ and π. The conductor Green's function is then

$$G(E) = [E - H_c - \Sigma_L(E) - \Sigma_R(E)]^{-1} = \frac{|0\rangle\langle 0|}{E - \epsilon_0 - 2\eta^2 V e^{-i|\theta|}}, \tag{26}$$

and the Γ matrices are

$$\Gamma_L(E) = \Gamma_R(E) = 2\eta^2 V \sin|\phi| |0\rangle\langle 0|. \tag{27}$$

The transmission is then

$$T(E) = \mathrm{Tr}\{\Gamma_L G \Gamma_R G^\dagger\} = \langle 0|\Gamma_L G \Gamma_R G^\dagger|0\rangle = \frac{\hbar^2 v^2(E)}{\frac{[E(1-\eta^2)-\epsilon_0]^2}{\eta^4} + \hbar^2 v^2(E)} \tag{28}$$

which is exactly what we obtained earlier in a different manner.

For the special case $\eta = 1$, we have

$$T(E) = |t|^2 = \frac{\hbar^2 v^2(E)}{\epsilon_0^2 + \hbar^2 v^2(E)} \tag{29}$$

Additionally, if $\epsilon_0 = 0$, the incoming wave is not scattered at all, and we have perfect transmission ($T = 1$). As $|\epsilon_0|$ is increased, the transmission everywhere decreases. At the band edges, $E = \pm 2V$, $\hbar v(E) = 0$ and the transmission vanishes (unless also $\epsilon_0 = 0$). The maximum transmission is at $E = 0$. The transmission when $\eta = 1$ is not sensitive to the sign of ϵ_0. The transmission as a function of energy for different values of $a \equiv \epsilon_0/2V$ is plotted in figure 2.

6.2 2-Level Conductor

Next, we have considered a conductor with two energy levels ϵ_A and ϵ_B. Both energy states are connected to both contacts with a strength V. The total Hamiltonian has again the form (16), except now with

$$H_c = \epsilon_A |A\rangle\langle A| + \epsilon_B |B\rangle\langle B| \tag{30}$$

$$\tau_L = V|A\rangle\langle -1| + V|B\rangle\langle -1| \tag{31}$$

$$\tau_R = V|A\rangle\langle +1| + V|B\rangle\langle +1| \tag{32}$$

where $|A\rangle$ and $|B\rangle$ are the two conductor states. The conductor Hamiltonians H_A and H_B are the same as in the previous section. Calculating the transmission (with the Green's function or otherwise) yields

$$T(E) = \frac{\hbar^2 v^2(E)}{\frac{(E^2 - \epsilon_A \epsilon_B)^2}{(2E - \epsilon_A - \epsilon_B)} + \hbar^2 v^2(E)}. \tag{33}$$

For the purpose of comparison with the result for the one level system with $\eta = 1$, equation (29), we have considered the case where the two conductor levels are degenerate, $\epsilon_A = \epsilon_B = \epsilon_0$. For the transmission this yields

$$T_2(E) = \frac{\hbar^2 v^2(E)}{\frac{(E + \epsilon_0)^2}{4} + \hbar^2 v^2(E)}. \tag{34}$$

The transmission again vanishes at the band edges. This result differs from the single level case above in that the transmission is no longer symmetric around $E = 0$, and it is also sensitive to the sign of ϵ_0. Furthermore if ϵ_0 is within the band ($|\epsilon_0| < 2V$), then at $E = -\epsilon_0$ the conductor becomes transparent ($T = 1$). In contrast, for the one level conductor with $\eta = 1$, the transmission is always less than 1 for $\epsilon_0 \neq 0$. The transmission as a function of energy is plotted in figure 3.

6.3 N-Level (Degenerate) Conductor

Next we considered a conductor consisting of N degenerate levels, with each level coupled to both contacts with an interaction strength V. The result for the transmission, a generalization of equation (34) is

$$T_N(E) = \frac{\hbar^2 v^2(E)}{\frac{[E(1-N) - \epsilon_0]^2}{N^2} + \hbar^2 v^2(E)}. \tag{35}$$

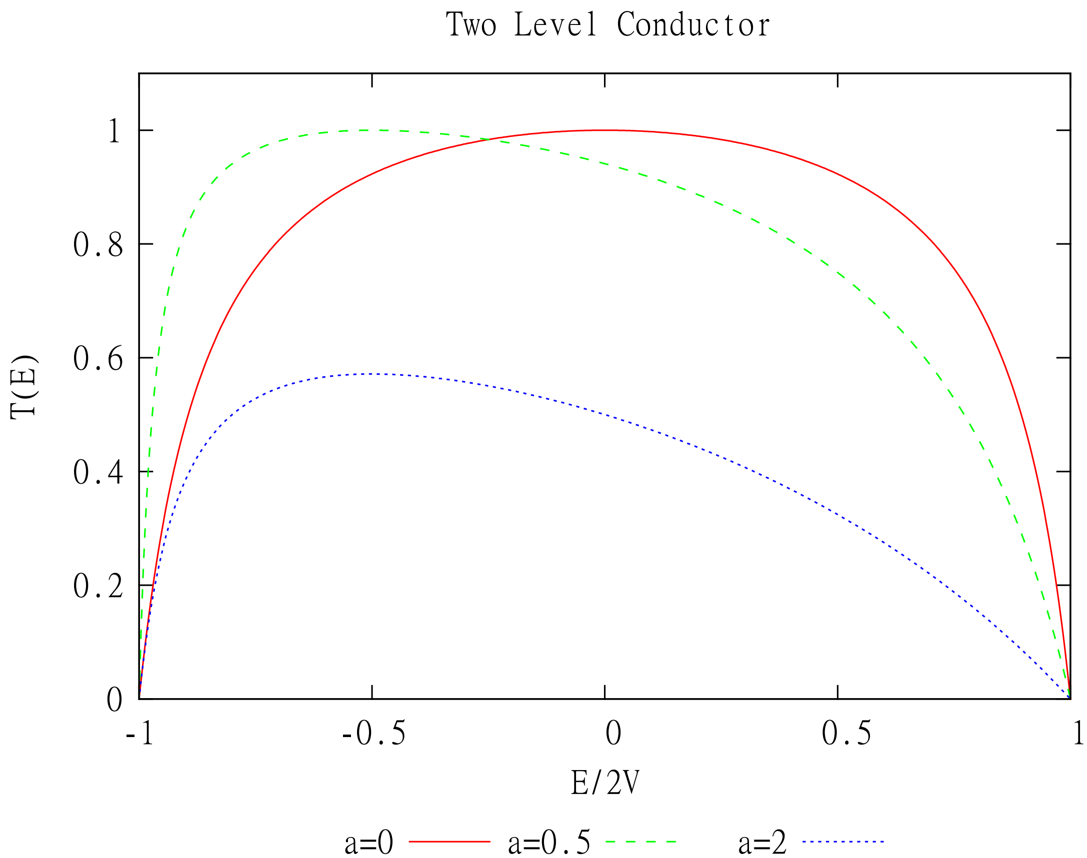

Figure 3: Transmission versus energy for the degenerate two level conductor for different values of $a \equiv \epsilon_0/2V$

Qualitatively, the behavior is similar to the two level case. $T_N(E)$ is again asymmetric around $E = 0$, and if ϵ_0 is within the band, the conductor is transparent at $E = \epsilon_0/(1-N)$. It is also interesting to note that this result is equivalent to equation (23) if we replace η^2 with N.

6.4 1-Level Conductor Interacting with a Harmonic Oscillator

Next we chose to look at a one level conductor which is interacting with a harmonic oscillator. This simplified system represents internal states of a conductor. For the total Hamiltonian we take

$$\begin{aligned} H = V \sum_{m=-\infty}^{\infty} (|m\rangle\langle m+1| + |m+1\rangle\langle m|) \otimes I_b + \epsilon_0 |0\rangle\langle 0| \otimes I_b \\ + I_e \otimes \hbar\omega \left(\frac{1}{2} I_b + b^\dagger b \right) + |0\rangle\langle 0| \otimes g\hbar\omega(b + b^\dagger) \end{aligned} \tag{36}$$

where the $|m\rangle$'s are the electronic states, b and $b^\dagger$ are the annihilation and creation operators for the bosons, I_b and I_e are the boson and electron identity operators, and g is a dimensionless constant which describes the strength of the interaction with the conductor state. The interaction between conductor and oscillator changes the effective energy of the $|0\rangle$ state based on the position of the oscillator.

Provided the temperature is low enough, the oscillator should be in its (non-shifted) ground state $|\phi_0\rangle$ before the electron passes through the junction, so for the incoming wave we take

$$\sum_{m<0} e^{ik_0 m}|m\rangle \otimes |\phi_0\rangle \tag{37}$$

where the energy of the incoming electron is $E_e = 2V\cos k_0$. Because of the interaction, as the electron passes through the conductor it may create one or more excitations in the oscillator, so the reflected and transmitted waves must be of the form

$$\text{reflected wave: } \sum_{m<0}\sum_{n} r_n e^{-ik_n m}|m\rangle \otimes |\phi_n\rangle \tag{38}$$

$$\text{transmitted wave: } \sum_{m>0}\sum_{n} t_n e^{-k_n m}|m\rangle \otimes |\phi_n\rangle \tag{39}$$

where r_n and t_n are reflection and transmission amplitudes for modes with n bosons in the oscillator. The $|\phi_n\rangle$'s are n boson eigenstates of the non-shifted oscillator. Since the incoming wave only has enough energy to create a finite number of bosons, some of the k_n's will necessarily be complex, and part of the electron wavefunction will be exponentially localized around the conductor.

Enforcing $H|\psi\rangle = E|\psi\rangle$ with $|\psi\rangle$ consisting of the sum of incoming, reflected, and transmitted waves, it is possible to show that the k_n's are determined by

$$E_{\text{total}} = 2V\cos k_0 + \frac{\hbar\omega}{2} = 2V\cos k_n + \hbar\omega\left(n + \frac{1}{2}\right) \tag{40}$$

and the reflection and transmission amplitudes are

$$\delta_{n,0} + r_n = t_n = -2iV\sin k_0 \langle\phi_n|G(E)|\phi_0\rangle \tag{41}$$

and the Green's function G is

$$G(E) \equiv [E - H_0 - H_1 - 2\Sigma(E)]^{-1} \tag{42}$$

with

$$H_0 \equiv \epsilon_0 + \hbar\omega\left(b^\dagger b + \frac{1}{2}\right), \tag{43}$$

$$H_1 \equiv g\hbar\omega(b + b^\dagger), \tag{44}$$

$$\Sigma(E) \equiv V\sum_n e^{ik_n}|\phi_n\rangle\langle\phi_n|. \tag{45}$$

If we consider the special case $\hbar\omega > 4V$, then the incoming electron does not have enough energy to create a boson and keep propagating, all k_n's for $n > 0$ will be complex, and the transmission is only affected by t_0,

$$T = |t_0|^2 = [2V\sin k_0]^2\langle\phi_0|G(E)|\phi_0\rangle\langle\phi_0|G^\dagger(E)|\phi_0\rangle. \tag{46}$$

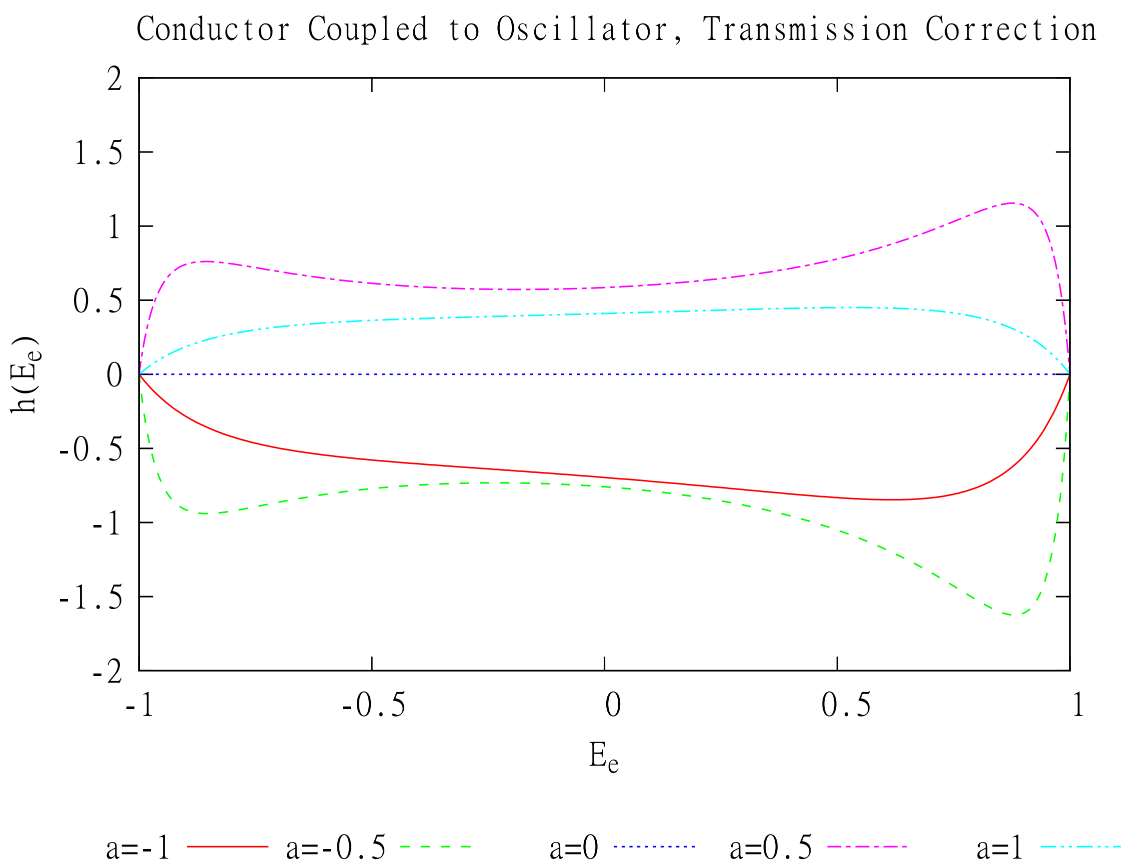

Figure 4: First order correction to transmission for a one level conductor interacting with an oscillator for different values of $a \equiv \epsilon_0/2V$ and with $\hbar\omega = 8V$.

Due to the difficulty in calculating $G(E)$ exactly, we have considered the limit of weak coupling g. Expanding equation (42), we have [36]

$$G = G_0 + G_0 H_1 G_0 + G_0 H_1 G_0 H_1 G_0 + \ldots \tag{47}$$

where

$$G_0(E) = [E - H_0 - 2\Sigma(E)]^{-1} = \sum_n \frac{|\phi_n\rangle\langle\phi_n|}{E - \epsilon_0 - \hbar\omega(n+1/2) - 2Ve^{ik_n}}. \tag{48}$$

Using this approximation, the transmission when $\hbar\omega > 4V$ to order g^2 is

$$T(E_e) \approx \frac{\hbar^2 v^2(E_e)}{\epsilon_0^2 + \hbar^2 v^2(E_e)} + g^2 h(E_e) \tag{49}$$

where the correction term is

$$h(E_e) \equiv \frac{2\epsilon_0 \hbar^2 \omega^2 \hbar^2 v^2(E_e)}{\left[\epsilon_0^2 + \hbar^2 v^2(E_e)\right]^2 \left[\epsilon_0 + \sqrt{\hbar^2\omega^2 - 2E_e\hbar\omega - \hbar^2 v^2(E_e)}\right]} \tag{50}$$

and with $v(E_e)$ again the velocity as a function of the electron energy, $\hbar^2 v^2(E_e) \equiv 4V^2 - E_e^2$.

This correction term may be positive or negative depending on the sign of ϵ_0, and it is not symmetric around $E_e = 0$. Interestingly, the $h(E_e)$ also vanishes if the site energy ϵ_0 is zero. The function $h(E_e)$ is plotted in figure 4.

7 Conclusions

We have examined quantum transport in nanowires with several different formalisms. The Boltzmann equation based theory of Lyo and Huang is able to incorporate many different kinds of scattering and make interesting predictions but we find absent in it a simple way of providing physical understanding of its effects. The STM theory of Kenkre, Biscarini, and Bustamante incorporates incoherent scattering in a much simpler way, but difficulties arise when the motion is fully coherent. Wigner functions, which are quasi-probability distributions defined on phase space, are appealing because of the conceptual similarity to classical transport theory. We were able to calculate the Wigner function for ballistic 1D conductors and show that the current reduces to the Landauer result, but incorporating boundary conditions correctly in more complicated cases remains a problem to complete. We have found the transmission formalism to be quite useful for simpler systems with elastic scattering when the motion is fully coherent and accordingly we have provided analysis of interactions of the conductor with a bath represented in a simple manner by harmonic vibrations.

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